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An Elementary Method for Averaging over Molecular orientations in the Calculation of Electron-Impact Ionization of Molecules JUN-FANG GAO, DON H. MADISON, JERRY L. PEACHER, Department of Physics of University of Missouri-Rolla — One of the difficulties associated with the calculation of fully differential cross sections (FDSC) for electron-impact ionization of molecules is that the experimental data typically do not resolve the orientation of the molecules which means that the theoretical approaches have to average over all orientations. This is not a problem for elementary approaches but it becomes an important constraint for more sophisticated approaches which require extensive computer time for a single orientation. A new method is proposed for averaging over molecular orientations which can be shown to be valid for gerade states if the S-basis function is dominate in the formation of the Molecular Orbital (MO). This method for averaging the orientations will be used to calculate FDSC in the DWIAOA (Distorted Wave Impulse Approximation Orientation Average) and 3DWOA (3- body Distorted Wave Orientation Average). Results will be presented for electron impact ionization of Hydrogen, Nitrogen and Water molecules over a wide range of incident-electron energies. The agreement with experimental data is good.

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